2599-Pos Board B618
Distance Estimation between Coarsened Regions of Biopolymers for Far Field Force Approximation
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Current strategies to simulate dynamic behavior of large molecular systems involve computationally expensive fully atomistic models, or lower resolution models that have been coarsened. Coarsening is accomplished by grouping tightly bonded atoms, with little relative motion, in two main ways: spherical beads, and rigid bodies. The latter method, which preserves system geometry, has been shown to better capture the system physics by including rotational equations of motion of the coarsened region. This can have a significant effect on the system dynamics. The most advanced of these methods adaptively determine the regions that should be coarsened, and approach O(log(n)) computational performance (n is the number of coarsened regions in the system). Low computational order methods are limited by the pairwise force computation at each time step, which is required for biochemical systems. Thus, an approximation has been proposed for use with these methods that reduce the computational complexity of the force computation to O(nlog(n)).
This approximation method (constructed similarly to the Fast Multipole Method) requires that the minimum distance between coarsened regions be computed. Intuitively obvious strategies, such as tracking the exact system geometry, are often so expensive that they negate the benefits of using a reduced order method. To this end, pseudo-radius of gyration is proposed that is computed from a tensor quantity similar to the inertia tensor, but describes the charge distribution of the coarsened region. The mechanisms for manipulating this quantity during the assembly and disassembly of coarsened regions would be similar to what is done for the actual inertia tensor in the current dynamics model. This quantity will be computationally inexpensive to store and manipulate, therefore will preserve the overall low computational cost of the force approximation, while allowing for a more accurate coarsening strategy.

2600-Pos Board B619
Application of Explicit-Solvent Constant ph Molecular Dynamics to Proteins
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Solution pH is a critical factor in biological and chemical processes. To enable molecular simulations of proton-coupled dynamics in these processes, the continuous constant pH molecular dynamics (CpHMD) method has been developed. Recently, we extended the CpHMD framework to explicit-solvent simulations and tested on the titration of a series of aliphatic dicarboxylic acids. Here we applied the method to several proteins including 36-residue HP36, 45-residue BBL, 56-residue NTL9, and 129-residue HEWL. The calculated pKa's have a root mean square deviation below one pH unit from experiment. This accuracy is comparable to the hybrid-solvent CpHMD, where the Generalized-Born (GB) implicit-solvent model is used to propagate titration coordinates while explicit-solvent is used to propagate conformational degrees of freedom. However, the explicit-solvent method avoids the artifacts and limitations of the GB model. This work demonstrates that the explicit-solvent CpHMD method paves the way for realizing pH-controlled all-atom MD simulations.

2601-Pos Board B620
Incorporating Protein Topology Information in Similarity Matrices for Improved Sequence Matching (A Fold-Specific Scoring System)
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Sequence matching is an important tool for much of biology. It is important for discovering information such as functional and evolutionary relationships. Functions for a large fraction of the genes identified today are unknown and gene annotation projects rely upon sequence matching.
Substitution matrices such as BLOSUM are widely used to find the sequence similarities. However, these matrices do not take into account structural information of proteins and treat all proteins classes the same. It is reasonable to hypothesize that use of structural information can lead to improvements in sequence matching. We have used CATH topologies where protein structures are clustered at 35% sequence identity. In the multiple sequence alignments, the number of times one amino acid is substituted by another is counted in order to obtain mutability matrices for each topology. These data are then combined with BLOSUM62 with a range of weight coefficients to obtain perturbed BLOSUM matrices for each topology.
A set of 27 sequence-dissimilar (less than 25% similarity) structurally-similar pairs of proteins that belong to unique CATH topologies were used as the test dataset. The sequence matching scores for all the sequence pairs in the test set along with scores for all the cross sequence pairs were calculated separately using (1) the BLOSUM62 matrix and (2) the corresponding new matrix for the topology of each sequence pair. Z-scores were used to compare the results obtained from the original BLOSUM and the perturbed matrices.
Improved sequence matching scores are obtained for 59% of the test cases.

Computational Methods II

2602-Pos Board B621
Competition between Adsorption and Intrinsic Collapse of Full-Length Aβ1-42 on the Surface of a Single-Walled Carbon Nanotube: Insights from Molecular Dynamics Simulations
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The ability of nanomaterials to interact with and influence biological macromolecules is increasingly gaining attention due to potential usages in therapeutic strategies. We have examined the interactions of the full length Aβ peptide monomer with the curved hydrophobic surface of a single walled nanotube using atomistic molecular dynamics simulations. Regardless of the initial orientation, the peptide rapidly adsorbs on the nanotube surface and results in disturbing the spontaneity of its own collapse. Detailed analyses of the energetics of the twin phenomena show that key interactions that are primarily responsible for the collapse are almost exactly compensated by interactions arising from the nanotube. We describe the cooperation between the central hydrophobic core and the N-terminal domain in bringing about complete adsorption. We further compare the relative influences of pure hydrophobicity and the π-π stacking propensity in the observed phenomena. The results indicate that nanomaterials such as carbon nanotubes may be useful in preventing key steps in Aβ self-assembly.

2603-Pos Board B622
Physical Effects Controlling Flock Formation in Systems of Self-Propelled Rods
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Collective motion occurs in a wide range of biological settings, including flocks of birds, swimming bacteria, and cytoskeletal filaments. Motivated by swimming microorganisms and filament motion in a motility assay, we study a simple model of self-propelled rods using Brownian dynamics simulations and analytic theory. A flock is a group of neighboring rods that move collectively. Because the physical interactions between the rods are purely repulsive, the formation of flocks requires nonequilibrium driving. We characterize the physical interactions controlling flock stability, internal flock structure, and the distribution of flock sizes. Quantifying the dynamic phases of the flocking system through measurement of correlation functions, order parameters, and stress tensor gives insight into the origin of flocking in a simplified model system.

2604-Pos Board B623
An Iterative Incompressible Immersed Boundary Method Applied to Biofluid-Structure Interaction Problems
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This work reports on the development of a novel iterative coupling between the Immersed Boundary method (IBM)[1] and a modified projection-based pressure correction, under the assumption of global incompressibility; its validation using a problem of practical interest - flow past an obstacle; and its application on the simulation of an idealised physiological system - blood flowing past a thrombotic-filter. Indeed, the method presented in [2] was improved through a Lagrangian restoring force based correction of the post-projection residual IB-velocity, which is inherent in fractional-step methods[3], being more evident at high Reynolds numbers Re. Overall, the results have shown that the proposed approach is very promising to study complex flow-structure interaction problems under the assumption of global incompressibility, which are commonly found in biophysical systems. The number of iterations remains almost constant

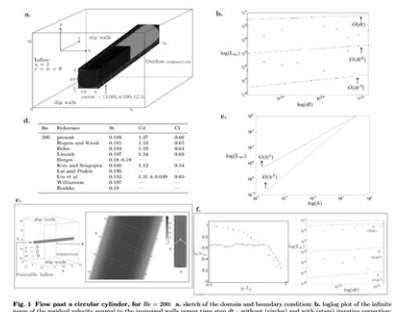

Fig. 1 Flow past a circular cylinder, for $Re = 200$**: a.** sketch of the domain and boundary condition; **b.** loglog plot of the infinite norm of the residual velocity normal to the immersed walls versus time-step dt - without (circles) and with (stars) iterative correction; **c.** loglog plot illustrating the achieved spatial convergence $O(h^2)$; **d.** values for lift and drag coefficients - Cl and Cd, along with Strouhal number St achieved in the present work and compared to numerical and experimental results from literature; *Ji et al* [C. Ji et al, J. Comput. Fluid Dynamics, 25-4, 207–221 (2011)], Uhlmann [M. Uhlmann, J. Comput. Phys. 209, 448–476 (2005)], Lai and Peskin [M. Lai and C. Peskin, J. Comput. Phys. 160:2, 705–719 (2000)], Liu et al [C. Liu et al, J. Comput. Phys. 139, 35–57 (1998)], Rashbi [A. Rashbi, NACA Rep.1191 (1954)], Frank et al [R. Franke et al, J Wind Eng Ind Aerodynamics, 35, 237–257 (1990)], Williamson [C. H. K.Williamson, Annual Review of Fluid Mechanics, 28, 477–539 (1996)], Lima e Silva et al [A. L. F. Lima e Silva et al, J. Comput. Phys, 189:2, 351–370 (2003)], Kalita and Sen [J. C. Kalita and S. Sen, J. Computers and Fluids, 59, 41–60 (2012)], Rogers and Kwak [S. E. Rogers and D. Kwak, AIAA Journal, 28:2, 253–262 (1990)], Belov [A. Belov et al, AIAA Journal, 95-0689 (1995)], Linnick [M. N. Linnick and H. F. Fasel, J. Comput. Phys, 204, 157–192 (2005)], Berger [E. Berger and R. Wille, Ann. Rev. Fluid Mech, 4, 313–340 (1972)], Kim and Sengupta [M. S. Kim and A. Sengupta, J. Mech. Science. And Technology, 19:3, 877–886 (2005)], and Williamson [C. H. K. Williamson, Phys. Fluids, 31, 2742–2744 (1988)]. **Blood flowing past a thrombotic filter, for** $Re = 1765$**: a.** sketch of the domain and boundary conditions; **b.** in the close up view the dimensionless streamwise velocity without (left) and with (right) an imposed thresholding-like, $z = L_z/2$, **f.** on the left, the velocity profile with (stars) and without (points) the thresholding-like, versus the analytical solution (circles) - $x = L_x/2$ and $z = L_z/2$; and on the right, the loglog plot of the infinite norm of the residual velocity normal to the immersed vessel and filter walls versus time step dt - without (circles) and with (stars) iterative correction. The parameters h and L_c represent mesh spacing and length in - direction, respectively while the notation $O(\cdot)$ reads comparison of order -, and the normalization factor U_∞ represents the freestream velocity. In terms of spatial analysis, the achieved spatial order of convergence agrees with the second order finite difference scheme being used and regarding temporal analysis, the proposed iterative correction resulted in a noticeable reduction in the maximum error and, as a consequence, the order of convergence of the second order Adams-Bashfort scheme being used was preserved.